

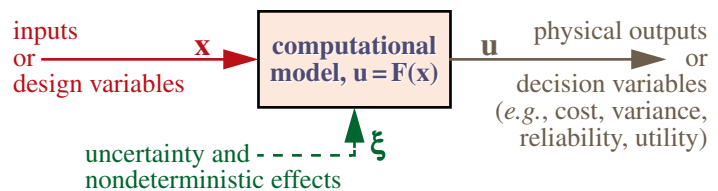
# DESIGN OF COMPUTER EXPERIMENTS USING DISCREPANCY SENSITIVITY

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**Extended Abstract:** Problems in uncertainty and optimization are widespread in science and engineering. Their use in simulation for studying complex dynamical systems, from real models of civil and aerospace structures to detailed models of weapons systems, is vital to design, analysis, and reliability characterization. Indeed, optimal design and superior reliability of key facilities and capabilities in the light of uncertain events and threats have been on the front pages of our morning newspapers in these days of seemingly impending war and concerns about international terrorism. Design and analysis of such systems is increasingly based on computer simulation, sometimes due to monetary, policy, or practical impediments to physical testing, but often due to the extreme complexity of the problems. Some examples of large-scale computational models of current and pressing interest are accident investigation of complex systems (space shuttle *Columbia*), climate modeling (NCAR's *Community Climate System Model*), projectile penetration into a media, protein and DNA/RNA modeling (pharmaceutical research), biomedical applications (human heart, bioelectrochemistry of the brain), cosmological models (early post-big-bang universe), etc. In all of these, model complexity and uncertainty abound.

Great strides have been made in computational ability in recent years, advanced by programs like the Accelerated Strategic Computing Initiative (ASCI, 2000) and through massively-parallel capable codes such as those in development at various national laboratories, *e.g.*, DAKOTA at Sandia National Laboratories (Eldred, 2001; Wojtkiewicz *et al.*, 2001). Yet, exacting study of the aforementioned complex systems, with all of the uncertainties that influence their behavior, taxes the computational capabilities of today's most advanced computer platforms. Models with billions of equations are quite conceivable today, and it is likely that the higher-fidelity models of tomorrow will challenge the computational resources that will be available in the near future. As a result, methods are required to select and choose which simulations will provide the most useful information given the limited number of simulations that can be performed. For systems with few inputs, it is often obvious by inspection where new sample points should be placed. In contrast, identifying empty regions of high-dimensional input/output spaces is a difficult task.

As a result, various methods have been advanced for the design of computer experiments (DoCE). The typical scenario is a computational model that maps a set of inputs to a set of outputs in deterministic or probabilistic fashion. The outputs can be physical quantities or derived functions like cost, utility, safety, reliability, mean, variance, etc. Some of the inputs could be design variables, and some of the outputs may be responses to be optimized by adjusting the inputs. In any case, when the computational model is very complex, it is infeasible to test all possible inputs and scenarios. This is true both for analyzing the forward problem to quantify the propagation of uncertainty as well as for design optimization. A number of approaches for choosing sample simulation points are in the literature.



**Figure 1. Uncertain computational input/output map.**

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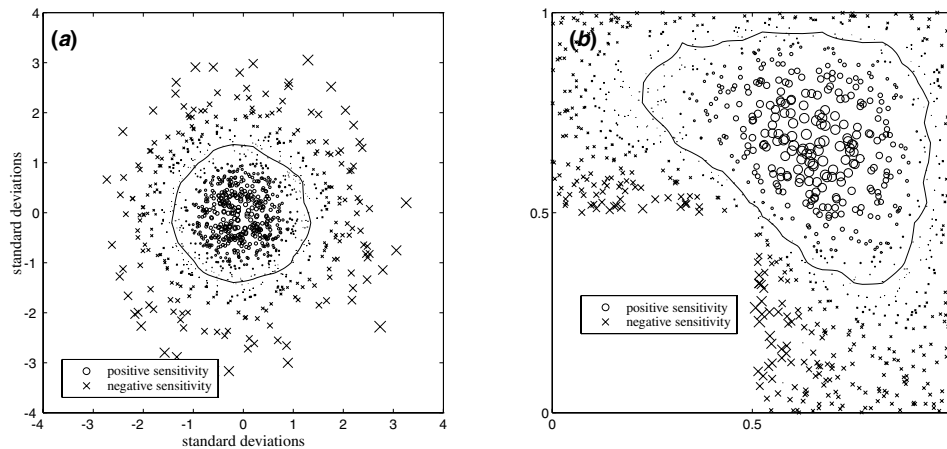
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Wynn (1970) and Mitchell (1974) give some of the early work for design of experiments for complex systems. Some common strategies for designing experiment inputs are Latin Hypercube sampling (McKay *et al.*, 1979; Imam and Conover, 1982; Imam and Shortencarier, 1984; Tang, 1993; Owen, 1994; Ye, 1998), orthogonal array sampling (Koehler and Owen, 1996), Monte Carlo and quasi-Monte Carlo methods (Niederreiter, 1992), etc. Conventional grid approaches place samples in a deterministic way in a regular grid of points. In Monte Carlo, samples are selected randomly according to their user-specified probability distributions. Latin Hypercube sampling (LHS), a form of stratified sampling (Hammersley and Handscomb, 1964), takes samples at random from distinct hypercubes in the input variable space. Quasi-Monte Carlo methods use sequences of inputs that are designed to fill the input sample space in a deterministic way.

The aim in designing an efficient set of computer experiments is to maximize the knowledge gained from a limited allocation of computational resources. This goal takes several interrelated forms for various applications: in response surface modeling, the goal may be minimal error in a surrogate approximation of the surface; in uncertainty quantification, one may wish to limit or minimize statistical properties of functions of the input and/or output random variables; in design optimization, minimizing some expected cost and, often, its variance are the targets. However, the approaches in the literature lack quantitative measures of how much new “information” is added by new sample points. Further, while these methods can operate on the *input* space, they generally cannot directly evaluate and enhance the uniformity of sample points in the *output* space.

Thus, this paper advances a new method, based on the mathematical definitions of *discrepancy* and *discrepancy sensitivity*, of quantifying the contribution of a given sample point to the uniformity of samples in the entire input/output domain. Discrepancy, which probably stems from the work of Kolmogorov (1933), is defined in a number of works in the literature (*e.g.*, Proinov, 1985; Niederreiter, 1992; Morokoff and Caflisch, 1994). Essentially, the various discrepancy definitions are measures of the error between a theoretical distribution and an empirical one based on a set of sample points. The sensitivity of the discrepancy with respect to the existence of a sample point was derived by Johnson (1997) and is also summarized in Johnson and Wojtkiewicz (2002). In the interests of brevity, these derivations are omitted here.

To show that the discrepancy sensitivity does indeed classify as “important” the sample points near holes in the sample space, consider two distributions of 1000 points each, as shown in Fig. 2. The sensitivities correctly indicate, with large negative sensitivities, that more samples should be added near the outer edges or “tails” of the Gaussian distribution and in the empty quadrant for the uniform

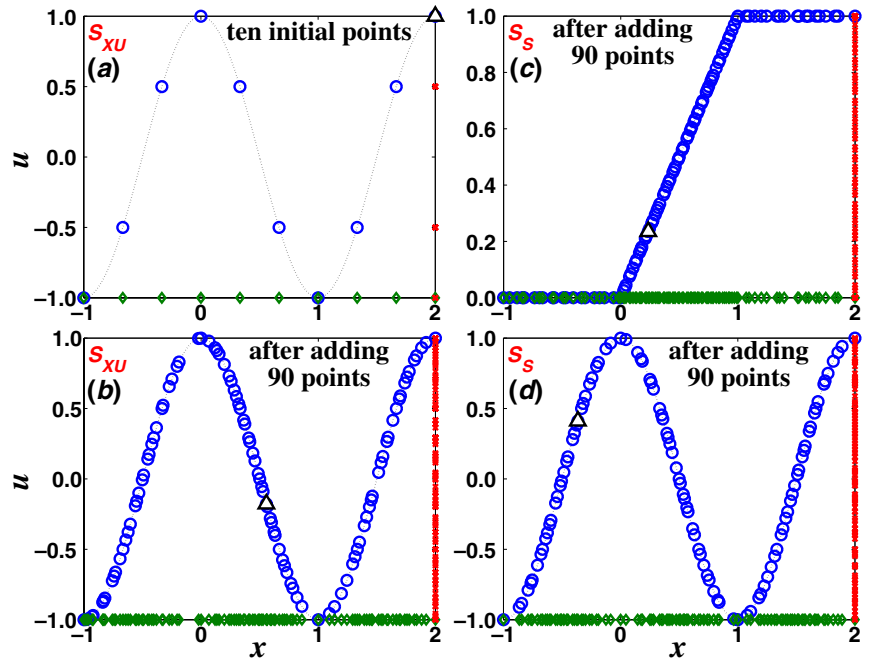


**Figure 2. Discrepancy sensitivity for 1000 sample points chosen (a) with a bivariate Gaussian distribution and (b) with a uniform distribution over three quadrants of the unit square.** The solid line represents an approximate contour of zero sensitivity. Marker sizes indicate sensitivity magnitude.

distribution with cutout. In Fig. 2a, the sensitivities near the mean are positive, indicating that extraneous samples are located there, and sensitivities in the “tails” are large negative values, implying that more samples should be added in the outer regions. This is exactly the type of indicator required for characterizing how well the space is filled in the vicinity of the sample points.

Some tests using discrepancy sensitivity to choose new points for characterizing and input/output maps have been performed. In these tests, single-input-single-output (SISO) maps were tested. While of low order and computationally trivial, these examples were chosen to represent some of the “difficult” behavior that often appears in real-world problems, such as multimodality, sharp corners and so forth. There are a number of discrepancy sensitivity measures that can be computed for input/output problems. For example, let  $\mathbf{x}$  be an  $n \times 1$  vector of inputs and  $\mathbf{u}$  be an  $m \times 1$  vector of outputs. The possible discrepancy sensitivity measures, then, include just that of the samples in the  $n$ -dimensional input space, just that of the samples in the  $m$ -dimensional output space, that of the combined  $(m+n)$ -dimensional combined input/output space, that of functions of inputs and outputs (*e.g.*, over the arc length for SISO and single-input-multi-output problems), etc.

To demonstrate, consider a ramp function with a sharply discontinuous slope and a multimodal cosine function, as shown in Fig. 3. In both cases, a set of ten sample points were first chosen with a grid approach, evenly distributed over the domain  $[-1, 2]$ , as shown in Fig. 3a. Ninety additional points are then added based on one of two sensitivity discrepancy measures. In Figs. 3a and 3b, the combined 2-dimensional input/output space discrepancy sensitivity is used. In Figs. 3c and 3d, the discrepancy sensitivity along the arc length is determined by using a piecewise linear curve through the points to determine arc length from the leftmost point.



**Figure 3. Sample point distribution (o) and the distributions projected just in the input space (◇) and just in the output space (x) for two different functions and two methods.**

In both cases, the discrepancy sensitivity is computed for all sample points, and then a cubic spline interpolant is used to find where the discrepancy sensitivity is most negative — the location to place a new point. This is carried out for each point added. The results are shown in Figs. 3b,c,d. It can be seen that both measures of sensitivity do provide coverage of the sample space in a relatively uniform manner.

In summary, this paper proposes a new approach for efficiently choosing sample points, based on the discrepancy sensitivity, for the design of computer experiments. This approach is grounded in the mathematical definitions of discrepancy, which are used in analyzing pseudorandom number generation and quasi-Monte Carlo methods. The long-term aim, as the authors continue to develop the discrepancy sensitivity method, is to develop the approach so that it can be incorporated into large-scale computational model simulations, and integrated into tools designed for performing the simulations such as DAKOTA (Eldred, 2001).

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